AD-A251 619

‖‖‖‖‖‖‖‖‖‖‖‖‖‖‖

[ATION PAGE

DATE	3. REPORT TYPE AND DATES COVERED
~~ May 1992	Technical 6/1/91–5/31/92

4. TITLE AND SUBTITLE

Comment on "Long–Range Spatial Self–Organization in the Adsorbate–Induced Restructuring of Surfaces: Cu{110}–(2x1)O"

5. FUNDING NUMBERS

6. AUTHOR(S)

J. A. Meyer, S. J. Stranick and P. S. Weiss

N00014–91–J–1630

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Department of Chemistry
152 Davey Laboratory
The Pennsylvania State University
University Park, PA 16802

8. PERFORMING ORGANIZATION REPORT NUMBER

Report #4

9. SPONSORING MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Office of Naval Research
Chemistry Program
800 N. Quincy Street
Alexandria, VA 22217-5000

DTIC
ELECTE
JUN 0 8 1992
S B D

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION AVAILABILITY STATEMENT

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

In a recent letter, Kern *et al.* reported that anisotropic Cu–O islands form striped periodic supergratings on the Cu{110} surface. Kern *et al.* attribute the formation of these striped phases to long–range repulsive forces between stripes. We have shown using Monte Carlo simulations and a 1–D Ising model that short range adsorbate–adsorbate interactions are capable of producing striped phases.

14. SUBJECT TERMS			15. NUMBER OF PAGES
			5 pages
			16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	UL

Comment on "Long–Range Spatial Self–Organization in the Adsorbate–Induced Restructuring of Surfaces: Cu{110}–(2x1)O"

J. A. Meyer, S. J. Stranick, and P. S. Weiss
Department of Chemistry
The Pennsylvania State University
University Park, PA   16802

In a recent letter [1], Kern *et al.* reported that anisotropic Cu–O islands form striped periodic supergratings on the Cu{110} surface. Kern *et al.* attribute the formation of these striped phases to long–range repulsive forces between stripes [1]. We have shown using Monte Carlo simulations and a 1–D Ising model that short range adsorbate–adsorbate interactions are capable of producing striped phases.

In the work of Kern *et al.*, the observed spacings between Cu–O islands depended upon the coverage and temperature, and were studied using scanning tunneling microscopy (STM) and He diffraction [1]. This work differed from earlier STM studies of this surface [2–5] in that the surface was annealed. The surface without annealing displays disordered "strings" of adsorbates along the <001> direction which are one atom wide in the <1$\bar{1}$0> direction [2–4], or islands of condensed strings [5]. Kern *et al.* found that annealed surfaces have "stripes" in the <001> direction which were several atoms wide and of quite uniform width and spacing.

Our sole purpose here is to demonstrate that short range adsorbate–adsorbate interactions are sufficient to reproduce the qualitative features observed for this interesting surface. We do not seek to extract specific interaction energies. Starting from randomly adsorbed O atoms on a Cu{110} surface at elevated temperature, we allow each adsorbate to move typically 10^6 times while cooling at a constant rate to room temperature. The main difference in the interaction energies in these simulations and those used in Ref. [4] is that we have added a weak adsorbate–adsorbate attraction for the next nearest neighbor site along the <1$\bar{1}$0> direction as suggested in Ref. [5].

We find for our simulations that upon cooling from 640K to 293K we form fairly evenly spaced stripes. The numbers and spacings of these stripes depend upon the coverage, but are the same for multiple runs at a given coverage. We find similar results for lattices of 30x30 and 60x60 Cu atoms, as well as for asymmetric lattices, all with periodic boundary conditions. We find that from *ca.* 8×10^4 up to *ca.* 10^7 moves per adatom, we obtain identical results. Fig. 1 shows the simulated stripe

92 6 05 055

spacing (D) *vs.* coverage which is in qualitative agreement with the experimental data — Fig. 2a of Ref. [1]. The vertical scale of this curve varies with the interaction energies chosen.

Randomly adsorbing O atoms at 294K, then allowing the same number of steps as for high temperature adsorption, results in disordered strings of adatoms as for some of the previous STM data [2–4] and as for the previous simulations [4], and also results in some two–dimensional growth as seen by STM in Ref. [5]. However, starting with one perfect stripe several atoms wide, we find that at 294K in 10^7 moves per adatom this island breaks up into the number of stripes found for the annealed surface at this coverage. We take this as evidence pointing toward the striped phases being equilibrium structures in our simulations.

By considering the strong adatom attraction in the <001> direction as the determining interaction in string formation, and the weaker adatom attraction in the <1$\bar{1}$0> direction as determining the string–string interactions, we have modeled the problem as a 1–D Ising model. Even in this simple model equally spaced bands are obtained with spacings and widths *vs.* coverage and temperature [6], in qualitative agreement with Fig. 2 of Ref. [1].

The essential qualitative features observed in the measurements of Kern *et al.* [1] on the O/Cu{110} surface have been reproduced using simulations which include only short range interactions including a weak adatom attraction in the <1$\bar{1}$0> direction. This is in contrast to the suggestion that long range forces need be invoked in order to explain this data [1]. Details of the calculations summarized above will be published shortly [6].

REFERENCES

1. K. Kern, H. Niehus, A. Schatz, P. Zeppenfeld, J. Goerge, and G. Comsa, *Phys. Rev. Lett.* **67**, 855 (1991).

2. D. J. Coulman, J. Witterlin, R. J. Behm, and G. Ertl, *Phys. Rev. Lett.* **64**, 1761 (1990).

3. F. Jensen, F. Besenbacher, E. Laensgaard, and I. Stensgaard, *Phys. Rev. B* **41**, 10233 (1990).

4. Y. Kuk, F. M. Chua, P. J. Silverman, and J. A. Meyer, *Phys. Rev. B* **41**, 12393 (1990).

5. J. Witterlin, R. Schuster, D. J. Coulman, G. Ertl, and R. J. Behm, *J. Vac. Sci. Technol. B* **9**, 902 (1991).

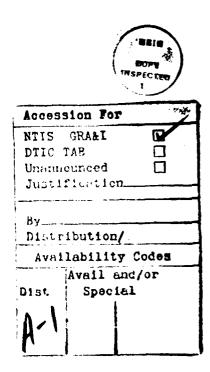6. J. A. Meyer, S. J. Stranick, J. H. Ferris, III, and P. S. Weiss, to be published.

FIGURE CAPTION

FIG. 1. Stripe spacing (D) *vs.* O atom coverage on the Cu{110} surface after cooling from 640K to 294K while allowing *ca.* 10^6 moves per adatom.